AR201-14132B

Substance Group:	**Group 2**
Summary Prepared by:	**Petroleum Additives Panel** **Health & Environmental Research Task Group**
Date of last update:	**December 16, 2002**
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1.0 Physicochemical Properties

Robust Summary #: 2-Physchem-1 (Boiling Point-Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling point calculated by MPBPWIN subroutine, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated BP (°C) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative 342 Benzene, C_{24} alkyl derivative 458 CAS# 68081-77-6 Benzene, C_{22} polypropene 388 Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene

	derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the boiling range of category members can range from 342 to 458°C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be >388°C for the polypropene derivative (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential boiling range for substances with the 2 CAS numbers listed under test substance.
Reference:	Boiling point calculated by MPBPWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Physchem-2 (Vapor Pressure Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure calculated by MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine method is described in: Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. The modified Grain method is described in: Neely and Blau's Environmental Exposure from Chemicals, Volume 1. 1985. CRC Press. Page 31.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated VP (Pa) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative $1.3e^{-2}$ Benzene, C_{24} alkyl derivative $1.7e^{-6}$ CAS# 68081-77-6 Benzene, C_{22} polypropene $6.2e^{-4}$ Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For

	example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the vapor pressure range of category members can range from $1.3e^{-2}$ to $1.7e^{-6}$ Pa at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be $<6.2e^{-4}$ Pa at 25 °C for the polypropene derivative (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential vapor pressure range for substances with the 2 CAS numbers listed under test substance.
Reference:	Melting point calculated by MPBPWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Physchem-3 (Water Solubility Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility calculated by WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated WS (mg/L) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative $2.0e^{-4}$ Benzene, C_{24} alkyl derivative $4.4e^{-9}$ CAS# 68081-77-6 Benzene, C_{22} polypropene 1.2^{-7} Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the

	benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the water solubility range of category members can range from $2.0e^{-4}$ to $4.4e^{-9}$ mg/L at 25 °C for the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) and can be $<1.2e^{-7}$ mg/L at 25 °C for the polypropene derivative (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential water solubility range for substances with the 2 CAS numbers listed under test substance.
Reference:	Water solubility values calculated by WSKOWWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Physchem-4 (Log Kow Range)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient estimations calculated by KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Substance Component — Calculated Log Kow CAS# 115733-08-9 Benzene, C_{14} alkyl derivative 8.9 Benzene, C_{24} alkyl derivative 13.8 CAS# 68081-77-6 Benzene, C_{22} polypropene 12.3 Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. The modeling data for physicochemical endpoints in Sections 2.2.5 to 2.2.7 are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight

	derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Modeling data indicate that the log of the octanol-water partition coefficients (log K_{ow}) for category members are estimated to be >8.9.
Reliability:	(2) Reliable with restrictions The results include calculated values based on chemical structure and represent a potential log Kow range for substances with the 2 CAS numbers listed under test substance.
Reference:	Log Kow values calculated by KOWWIN subroutine, which is contained in the computer program: EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

2.1 Hydrolysis

Robust Summary #: 2-Hydro-1

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group

	(HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of chemicals in the Arylpolyolefin Category. Two CAS numbers identify substances in this category: • 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • 68081-77-6; Benzene polypropene derivatives As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur. The Arylpolyolefin Category Commercial arylpolyolefins are manufactured by reacting anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. Linear alkylbenzenes use linear alpha olefins with $AlCl_3$ and HF as the preferred catalyst. Branched alkylbenzenes start with a tetrapropenyl (C_3) stream using HF as the preferred catalyst, but triethyl aluminum ($AlEt_3$) has also been used as a catalyst. Commercial substances in this category have a carbon number distribution between C20 to C30 or C28 to C88. The chemical constituents of these substances are composed of carbon and hydrogen and share a similar structure; they are linear or branched alkyl benzenes with alkyl groups ranging between C14 and C82. Because of their chemical similarity, this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Arypolyolefin. **Hydrolysis of Hydrocarbons as a Function of Molecular Structure** Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (1,2). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

	The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons are not subject to hydrolysis (2) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.
	Under strongly acidic conditions a carbon-carbon double bond can react with water by an addition reaction mechanism (1). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (2). Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (3). The chemicals in this category are arylpolyolefins that contain double bonds in the aromatic ring. The remaining chemical structure contains saturated hydrocarbons (paraffins). These chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Arylpolyolefin Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment. <u>References</u> 1. Gould, E.S. 1959. Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 2. Harris, J.C. 1982. "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 3. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	Not applicable
Reference:	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group. 2002. Hydrolysis: Arylpolyolefin Category. Rosslyn, VA, USA.

Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "hydrolysis". Selecting this option refers the reader to information in the "freetext" field for "test substance".

2.2 Photodegradation (Direct & Indirect)

Robust Summary #: 2-Photo-1 (Direct)

Test Substance*:	Other TS
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Test Substance:	CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (1). 1. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from**	Not applicable

guideline or protocol	
Direct Photolysis: • **Results: half-life, % degrad., quantum yield**	Not applicable
Indirect Photolysis: • **Results: type of sensitizer, concentration of sensitizer, rate const., % degrad., half-life**	Not applicable
Degradation Products: • **Note: Identification, concentration**	Not applicable
Conclusion:	**Technical Summary** In the environment, direct photolysis will not contribute to the degradation of constituent chemicals of substances in the Arylpolyolefin Category. Two CAS numbers identify substances in this category: • 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • 68081-77-6; Benzene polypropene derivatives The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (1). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state. The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (1). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule. The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (1).

	Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.
Conclusion: (continued)	A conservative approach to estimating a potential photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (2). Saturated hydrocarbons do not absorb light above 200 nm. Therefore, those constituents of substances in this category will not exhibit photolytic degradation. Single ring aromatics do not absorb sufficient light energy above 290 nm to cause photolysis (1). Therefore, the arylpolyolefins in this category are also not subject to photolytic processes. References 1. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 2. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
Reliability:	Not applicable
Reference:	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group. 2002. Hydrolysis: Arylpolyolefin Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the Test Substance pick list within the IUCLID data entry field for Photodegradation (direct). Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Photo-2 (Indirect)

Test Substance*:	Other TS
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis: • **Results: half-life, % degradation, quantum yield**	Not applicable
Indirect Photolysis: • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-life is normalized for a 12-hour day.

	Calculated* OH- Rate Constant Substance Component half-life (hrs) (cm^3/molecule-sec) CAS# 115733-08-9 Benzene, C_{14} alkyl derivative 5.67 23e-12 Benzene, C_{24} alkyl derivative 3.49 37e-12 CAS# 68081-77-6 Benzene, C_{22} polypropene 4.10 31e-12 * Atmospheric half-life values are based on a 12-hr day. Commercial substances in this category have a carbon number distribution between C20 and C30 or C28 and C88. The three chemicals selected to represent the atmospheric oxidation potential range of this category include a C20, C30, and C28 arylpolyolefin that have common structures. Calculated air oxidation potential values are presented as ranges for category members, where possible, and are based on the highest and lowest molecular weight derivative in each member. For example, structures representing the C_{14}-C_{24} alkaryl derivative (CAS # 115733-08-9) include a benzene C_{14} alkyl derivative and a benzene C_{24} alkyl derivative. Whereas, structures representing the polypropene derivative (CAS # 68081-77-6) include only the benzene C_{22} polypropene lowest molecular weight derivative; the benzene C_{82} polypropene highest molecular weight derivative has not been modeled as the molecular weight of this derivative falls outside of the applicable range of the EPIWIN modeling program. References 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. **7**:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., New York, NY, USA. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals

	and ozone. Chemosphere. **12**:2293-2299.
Degradation Products: • **Note: Identification, concentration**	Unknown
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (4). 4. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Atmospheric oxidation can contribute to the degradation of substances in this category. However, their low vapor pressures suggest that constituents of these substances will not partition to a great extent into the air phase where this reaction takes place. Therefore, this degradation process is not expected to significantly contribute to the degradative loss of these substances in the environment. Based on calculated values, substances in this category can have an atmospheric half-life range of 3.5 to 5.7 hours. These data suggest that the fraction of constituents that do partition to the air phase will degrade rapidly. These data represent a key study for characterizing the atmospheric oxidation potential of the Arylpolyolefin Category, which includes benzene C_{14}-C_{24} alkyl derivatives (CAS # 115733-08-9) and benzene polypropene derivatives (CAS # 68081-77-6).
Reliability:	(2) Reliable with restrictions The results include values calculated using the AOPWIN program and represent a potential atmospheric half-life range for substances with the 2 CAS numbers listed under test substance.
Reference:	Meylan, M., SRC. 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation

	Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".

Robust Summary #: 2-Fugacity-1

Test Substance*:	Other TS
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physical properties used with the model were calculated by the EPIWIN Estimation v 3.04 program (1). Output data from the equilibrium model provide basic information on the potential distribution of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	The following chemicals are representative of the two CAS numbers in the Arylpolyolefin Category, each of which contains complex, multi-constituent substances. The partitioning data characterize the range of constituent chemicals in each substance as well as the overall partitioning behavior of these substances. Calculated* Percent Distribution Substance Component — Soil — Sediment CAS# 115733-08-9 Benzene, C_{14} alkyl derivative — 97.7 — 2.17 Benzene, C_{24} alkyl derivative — 97.7 — 2.17

	CAS# 68081-77-6 Benzene, C_{22} polypropene97.7 2.17 Benzene, C_{82} polypropene97.8 2.17 * Distribution values determined using input data calculated by the EPIWIN program.
Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Distribution of representative chemicals to each remaining compartment (air, water, suspended sediment, biota) was calculated as less than 0.2%. Potential for mobility throughout the environment is expected to be low due to the relatively high log Kow values and low water solubility of constituent chemicals. Commercial substances in this category have a carbon number distribution between either C20 and C30 or C28 and C88. The four chemicals selected to represent the transport / distribution range of this category include a C20, C30, C28, and C88 arylpolyolefin that have common structures and represent the potential range of data for the two category substances.
Test Substance:	• CAS# 115733-08-9; Benzene C_{14}-C_{24} branched and linear alkyl derivatives • CAS# 68081-77-6; Benzene polypropene derivatives Arylpolyolefins are manufactured by mixing anhydrous alkylate (linear or branched) with benzene in the presence of catalyst and heat. More information on the Arylpolyolefin Category can be found in the American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group, High Production Volume test plan for this category (2). 2. Health, Environmental, Regulatory, Task Group (HERTG). 2002. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Arylpolyolefin Category. American Chemistry Council, Petroleum Additives Panel, HERTG.
Conclusion:	Substances in the Arylpolyolefin Category are expected to distribute primarily to soil with a small percentage partitioning to sediment. These data represent a key study for characterizing the fugacity of the Arylpolyolefin Category, which includes benzene C_{14}-C_{24} alkyl derivatives (CAS # 115733-08-9)

	and benzene polypropene derivatives (CAS # 68081-77-6). Comparatively, their potentials to partition in the environment are expected to be similar, based on their high log Kow and low water solubility values.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include estimated values calculated by the EPIWIN program based on chemical structure. The partitioning data represent a potential distribution range for substances in the two CAS numbers listed under test substance. Computer modeling is an accepted method of assessing environmental distribution of chemicals.
Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council; Petroleum Additives Panel; Health, Environmental, Regulatory, Task Group

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "transport / distribution". Selecting this option refers the reader to information in the "freetext" field for "test substance".

4.1 Acute Toxicity

4.1.1 Acute Oral Toxicity

Robust Summary #: 2-Acute Oral-1

Test Substance	
CAS #	CAS# 115733-08-9
Chemical Name	Benzene C14-C24 alkyl derivatives
Remarks	Test material dosed as received, purity not provided.
Method	
Method/Guideline followed	FHSA 16CFR1500.3
Test Type	Acute oral toxicity
GLP (Y/N)	N
Year (Study Performed)	1978
Species/Strain	Rats/ Sprague-Dawley strain
Sex	Male/Female
No. of animals/dose	5/sex
Vehicle	Corn oil
Route of administration	Oral (intragastric)
Dose level	5 g/kg
Dose volume	10 ml/kg
Control group included	No
Remarks field for test conditions	A single dose of the test material was administered intragastrically to five fasted male and female rats at each treatment level. The animals were observed for signs of toxicity or behavioral changes during the 4 hours post dosing and daily thereafter. Individual weights were recorded on the day of dosing, on day 7 and at termination. All animals were euthanized at the conclusion of the observation period. Gross autopsies were performed on all animals after 14 days.
Results	LD50 > 5 g/kg (males and females)
Remarks	All animals survived the duration of the study. Two males and two females were hypoactive at 1 hour post dosing and two females exhibited urine staining of the fur at 4 hours post dosing. All animals exhibited progressive body weight gains at each weighing interval. At necropsy one male exhibited an enlarged spleen and one female exhibited hydrometra of the uterus.
Conclusions	The test article, when administered to male and female Sprague-Dawley rats, had an acute oral LD50 of >5 g/kg.
Data Quality	Reliable without restriction (Klimisch Code).
References	Unpublished confidential business information
Other	Updated: 1/21/02

Robust Summary #: 2-Acute Oral-2

Test Substance	
CAS #	CAS# 68081-77-6
Chemical Name	Benzene, polypropene derivatives
Remarks	Test material dosed as received, purity not provided.
Method	
Method/Guideline followed	43 CFR 37336, 163.81-1
Test Type	Acute oral toxicity
GLP (Y/N)	Y
Year (Study Performed)	1980
Species/Strain	Rats/Sprague-Dawley strain
Sex	Male/Female
No. of animals/dose	5/sex
Vehicle	None
Route of administration	Oral (intragastric)
Dose level	5g/kg
Dose volume	6.35 ml/kg
Control group included	No
Remarks field for test conditions	A single dose of the undiluted test material was administered intragastrically to ten fasted (over night) animals at a dose level of 5 g/kg. A control group was not included. The animals were observed for signs of toxicity or behavioral changes twice daily. Individual weights were recorded on the day of dosing and on days 7 and 14. All animals were euthanized at the conclusion of the observation period. Gross autopsies were performed on all animals after 14 days.
Results	LD50 >5g/kg (males and females)
Remarks	All of the treated animals survived the duration of the study. One male exhibited wheezing at 1 to 4 hours post dosing. Three males and all of the females exhibited urine soaked fur through day 1 on test. No other abnormal clinical signs were observed. All animals gained body weight during the study. No treatment related gross postmortem findings were evident at necropsy.
Conclusions	The test article, when administered as received to male and female Sprague-Dawley rats, had an acute oral LD50 >5g/kg.
Data Quality	Reliable without restriction (Klimisch Code)
References	Unpublished confidential business information
Other	Updated: 1/21/02

4.1.2 Acute Dermal Toxicity

Robust Summary #: 2-Acute Dermal-1

Test Substance	
CAS #	CAS# 115733-08-9
Chemical Name	Benzene C14-C24 alkyl derivatives
Remarks	Test material purity not provided
Method	
Method/Guideline followed	OECD Test Guideline 402
Test Type	Acute dermal toxicity (Limit Test)
GLP (Y/N)	Y
Year (Study Performed)	1980
Species/Strain	Rabbits/New Zealand White
Sex	Male and female
No. of animals/sex/group	5
Vehicle	None
Route of administration	Dermal
Dose level	2 g/kg
Dose volume	2.3 ml/kg
Control group included	No
Remarks field for test conditions	Approximately 24 hours prior to topical application of the test material, the hair of each animal was closely clipped. The skin was not abraded. A single dose of 2 g/kg of the undiluted test material was administered dermally to five male and female animals. The test material was kept in contact with the skin for a period of 24 consecutive hours under a surgical dressing and plastic film. The application site was wiped clean of residual test material at the end of the 24-hour exposure period using saline. The animals were observed frequently for clinical signs on the day of dosing and once daily for 14 days after treatment. Individual body weights were recorded on the day of dosing and on days 7 and 14. Gross necropsies were performed on all animals on Day 14
Results	LD50 > 2.0 g/kg (males and females)
Remarks	No mortality was observed. The mean body weight of the males increased slightly during the study. The mean body weight of the females was unchanged during the study. Dermal irritation (erythema and edema) was observed in all rabbits and persisted at least 4 days post dosing. No treatment related gross necropsy effects were evident.
Conclusions	The test article, when administered dermally as received to 5 male and 5 female New Zealand white rabbits had an acute dermal LD50 of greater than 2.0 g/kg.
Data Quality	Reliable without restriction (Klimisch Code).
References	Unpublished confidential business information
Other	Updated: 1/21/02

Robust Summary #: 2-Acute Dermal-2

Test Substance	
CAS #	CAS# 68081-77-6
Chemical Name	Benzene, polypropene derivatives
Remarks	Test material purity not provided
Method	
Method/Guideline followed	43 CFR 37336, 163.81-2
Test Type	Acute dermal toxicity (Limit Test)
GLP (Y/N)	Y
Year (Study Performed)	1980
Species/Strain	Rabbits/New Zealand White
Sex	Male and female
No. of animals/sex/group	5
Vehicle	None
Route of administration	Dermal
Dose level	2 g/kg
Dose volume	2.54 ml/kg
Control group included	No
Remarks field for test conditions	Approximately 24 hours prior to topical application of the test material, the hair of each animal was closely clipped. Immediately prior to dosing the skin was abraded. A single dose of 2 g/kg of the undiluted test material was administered dermally to five male and female animals. The test material was kept in contact with the skin for a period of 24 consecutive hours under an elastic bandage. The application site was wiped clean of residual test material at the end of the 24-hour exposure period. The animals were observed for abnormal clinical signs twice daily for 14 days after treatment. Skin condition was evaluated daily. Individual body weights were recorded on the day of dosing and on days 7 and 14. Gross necropsies were performed on all animals on Day 14
Results	LD50 > 2.0 g/kg (males and females)
Remarks	No mortality was observed. All animals gained weight during the study. No abnormal clinical signs were observed during the study. One male exhibited slight and moderate erythema and one female exhibited slight erythema during the study. These animals also exhibited desquamation. No treatment related gross necropsy effects other than skin effects were evident.
Conclusions	The test article, when administered dermally as received to 5 male and 5 female New Zealand white rabbits had an acute dermal LD50 of greater than 2.0 g/kg.
Data Quality	Reliable without restriction (Klimisch Code).
References	Unpublished confidential business information
Other	Updated: 1/21/02

5.0 Genetic Toxicity

Robust Summary #: 2-GenTox-1

Test Substance	
CAS #	CAS# 115733-08-9
Chemical Name	Benzene C14-C24 alkl derivatives
Remarks	Test material purity not provided.
Method	
Method/Guideline followed	OECD Guideline 471
Test Type	Bacterial Reverse Mutation Assay
GLP (Y/N)	Y
Year (Study Performed)	1981
Test System	**Salmonella typhimurium**
Strains Tested	*Salmonella typhimurium* tester strains TA98, TA100, TA1535, TA1537, TA1538
Exposure Method	Plate incorporation
Test Substance Doses/concentration levels	0.025, 0.075, 0.25, 0.75 and 2.5 mg/plate with and without activation
Metabolic Activation	With and without (S9 fraction mix of livers of Aroclor 1254 pretreated Sprague Dawley rats)
Vehicle	Ethyl acetate
Tester strain, activation status, Positive Controls and concentration level	TA98 +S9 2-aminoanthracene 5 ug/plate TA98 -S9 2-nitrofluorene 5 ug/plate TA100 +S9 2-aminoanthracene 5 ug/plate TA100 -S9 sodium azide 30 ug/plate TA1535 +S9 2-aminoanthracene 5 ug/plate TA1535 -S9 sodium azide 30 ug/plate TA1537 +S9 2-aminoanthracene 5 ug/plate TA1537 -S9 9-aminoacridine 10 ug/plate TA1538 +S9 2-aminoanthracene 5 ug/plate TA1538 -S9 2-nitrofluorene 5 ug/plate
Vehicle Control	Ethyl acetate
Statistical Analysis	Mean revertant colony count and standard deviation were determined for each dose point.
Dose Rangefinding Study	No
S9 Optimization Study	No
Remarks field for test conditions	This study was conducted prior to the development of OECD Guideline No. 471. This study deviates from the guideline in that Tester Strain TA 1538 is not called for in the guideline but it was included. In addition E. coli WP2 urvA Tester Strain called for in the guideline was not include. There were two treatment sets for each tester strain, with (+S9) and without (-S9) metabolic activation. Each of the tester strains was dosed with five concentrations of test substance, vehicle control, and a positive control. Three plates/dose

	group/strain/treatment set were evaluated. 50-100 ul of test material, positive control or vehicle control were added to each plate along with 100 ul of tester strain, S9 mix (if needed) and 2.0 ml of top agar. This was overlaid onto the surface of minimal bottom agar in a petri dish. Plates were incubated for 48 hours at 37°C. The numbers of revertant colonies were counted with an automated colony counter. The test material was considered a mutagen if a dose related increase was found in the number of revertant colonies and if the first dose level considered for the increase had an average number of revertant colonies that was three times that of the vehicle control.
Results	The test substance was not genotoxic in this assay with or without metabolic activation.
Remarks	All data were acceptable and no positive increases in the number of revertants/plate were observed with any of the tester strains with or without metabolic activation. The positive control for each respective test strain exhibited an appropriate response (with or without S9) over the mean value of the vehicle control for a given strain, confirming the expected positive control response.
Conclusions	Under the conditions of this study, the test material was not mutagenic.
Data Quality	Reliable with restriction (Klimisch Code). Restriction due to the lack of any information regarding the selection of dose levels used during the study. In addition no information is presented regarding cytotoxicity or the presence of test material precipitate in the cultures.
References	Unpublished confidential business information
Other	Updated: 10/24/2002